Magnetic Linear X-Ray Dichroism as a Probe of the Magnetocrystalline Anisotropy

Gerrit van der Laan
Daresbury Laboratory, Warrington WA4 4AD, United Kingdom
(Received 15 June 1998)

We show that for itinerant $3d$ transition metal systems the magnetocrystalline anisotropy energy is directly related to the anisotropic part of the spin-orbit interaction, rather than to the orbital part of the magnetic moment as was previously suggested. We further show how the spin-orbit anisotropy can be obtained by applying the sum rule for magnetic linear dichroism in x-ray absorption. This provides an element specific tool to study metallic multilayer systems displaying novel magnetic properties, such as perpendicular magnetic anisotropy. [S0031-9007(98)08258-1]

PACS numbers: 75.30.Gw, 75.25.+z, 75.70.–i, 78.70.Dm

Although the microscopic origin of the magnetic anisotropy has been studied for the last six decades [1,2], interest has recently been revived by the advent of artificially made multilayers exhibiting perpendicular magnetic anisotropy (PMA). These layered structures, where each layer consists of different metals with a thickness of a few atomic layers, display a quasi-2-dimensional behavior. Anisotropy in the chemical bonding and crystalline structure leads to different in-plane versus out-of-plane properties which modify the magnetic moments. The preferred magnetization direction changes from in-plane to perpendicular when the magnetocrystalline anisotropy energy (MAE) is strong enough to overcome the shape anisotropy arising from the dipole-dipole interaction between the individual magnetic moments. The large MAE is attributed to the symmetry breaking at the interfaces, which partially removes the quenching of the spin-orbit interaction normally occurring in bulk transition metals.

The behavior of the magnetic moments in $3d$ transition metals with respect to the structural properties is primarily controlled by the small component ($\sim$10%) arising from the orbital part of the wave function. Using second-order perturbation theory Bruno [3] showed that the MAE can be related to the expectation value of the orbital moment $\langle L \rangle$. This model was corroborated by Weller *et al.* [4] who measured the anisotropy of the orbital moment with magnetic circular x-ray dichroism (MCXD). However, the observed orbital moment has to be scaled down in order to match value of the MAE. The issue continues to be of great interest, also because the technological importance is high.

In this Letter we propose a radically different way to obtain the element-specific MAE, namely by using magnetic linear x-ray dichroism (MLXD). Although MLXD has been recognized for its potential to measure besides ferro- and ferrimagnets also antiferromagnets, there have been few reports [5–8] compared to hundreds of MCXD studies. This might be due to the fact that it is not generally known what information is actually contained in the MLXD spectrum. It is often mentioned that one measures the square of the magnetic moment, i.e., $\langle M^2 \rangle$. However, this seems to be quite a crude portrayal of its capabilities, especially if we compare this to MCXD where application of the sum rules enables a precise description in terms of orbital and spin magnetic moments. A detailed specification of $\langle M^2 \rangle$ in the case of MLXD is therefore highly desirable. Another open question is the actual size of the MLXD signal. If MCXD is proportional to $\langle M \rangle$ and MLXD is proportional to $\langle M^2 \rangle$ then why is the latter effect so much smaller in $3d$ transition metals? In this Letter we will show that the MAE can be directly related to the anisotropic spin-orbit interaction and by using the results from the sum rules for linear dichroism we can develop a practical tool to study the anisotropic magnetic properties of multicomponent heteromagnetic systems.

The expectation value of the spin-orbit interaction in $3d$ transition metals can be obtained with perturbation theory because the spin-orbit constant is between 40 and 80 meV, which is small compared to the $3d$ bandwidth of a few eV. If we assume an unperturbed state $|s\rangle$ with energy ϵ_s, which mixes with excited states $|k\rangle$ due to the interaction $\lambda\zeta_l$, where $\lambda \equiv l \cdot s$ and ζ_l are the angular and radial part, respectively, of the spin-orbit operator for the l shell, the change in the ground state wave function is, in first order, given as

$$|s'\rangle = \sum_{k \neq s} \frac{\langle k|\lambda\zeta_l|s\rangle}{\epsilon_s - \epsilon_k} |k\rangle . \tag{1}$$

The expectation value of λ up to second order is

$$\begin{aligned} \langle \lambda \rangle &= \langle s + s'|\lambda|s + s'\rangle \\ &= \langle s|\lambda|s\rangle + 2\sum_{k \neq s} \frac{\zeta_l |\langle s|\lambda|k\rangle|^2}{\epsilon_s - \epsilon_k} + \ldots . \end{aligned} \tag{2}$$

Comparison of Eq. (2) with the energy calculated in a similar perturbation scheme yields

$$\zeta_l \langle \lambda \rangle = \epsilon_s^{(1)} + 2\epsilon_s^{(2)} + \ldots , \tag{3}$$

where $\epsilon_s^{(n)}$ is the nth order correction to the energy. In itinerant $3d$ transition metals the first-order term usually vanishes [9], so that

$$\epsilon_s^{(2)} = \tfrac{1}{2}\, \zeta_l \langle \lambda \rangle . \tag{4}$$

 0031-9007/99/82(3)/640(4)$15.00

When all d holes are in the minority spin band, such as in a "hard" ferromagnet, we can substitute $\langle\lambda\rangle = -\frac{1}{2}\hat{\mathbf{S}}\cdot\langle L\rangle$, where $\hat{\mathbf{S}}$ is the unit vector along the spin direction, and Bruno's formula [3] is retrieved,

$$\epsilon_s^{(2)} = -\tfrac{1}{4}\zeta_l\hat{\mathbf{S}}\cdot\langle L\rangle, \tag{5}$$

giving the relation between the MAE and the orbital moment. Whereas the left and right hand sides of Eq. (4) are invariant for symmetry operations of the lattice, this is not the case for Eq. (5), where the energy has different transformation properties than the projected orbital moment. Because of time reversal symmetry the orbital moment changes sign when the spin direction is reversed, which means that $\epsilon_s^{(2)} = -\frac{1}{4}\zeta_l\hat{\mathbf{S}}\cdot[\langle L^{\uparrow}\rangle - \langle L^{\downarrow}\rangle]$. However, the projected orbital moment measured with MCXD is $\hat{\mathbf{S}}\cdot[\langle L^{\uparrow}\rangle + \langle L^{\downarrow}\rangle]$, so that Eq. (5) becomes inadequate when there are also holes in the majority spin band. Furthermore, as pointed out by Wang *et al.* [9] the orbital moment operator acts only between states that conserve the spin and therefore cannot account for the spin-flip excitations from the occupied to unoccupied states near the Fermi level. Therefore, Eq. (4) is better suited to describe the MAE, but to turn it into practical benefit we require, of course, a measurement that gives the spin-orbit interaction. It is well known that by using the sum rule for the isotropic x-ray absorption spectrum the ground state spin-orbit interaction can be obtained from the branching ratio of the spin-orbit split core level edges [10]. However, in practice the isotropic spectrum is rarely measured, since the x rays are either linearly or circularly polarized. An extension of this sum rule to MLXD has been given by Carra *et al.* [11], and further generalized to resonant magnetic scattering by Luo *et al.* [12]. These theoretical studies give the result in a general form which is suited as a starting point of our treatment.

We consider an atom in an arbitrary ground state, where an electron from a core shell c is excited by electric dipole radiation into a partly occupied valence shell l. The core level is split by spin-orbit interaction into the levels $j_{\pm} = c \pm \frac{1}{2}$. We assume that there is no spectral weight transfer due to core-valence interactions, i.e., j is a good quantum number and also that the radial-matrix element is constant over each $j_{\pm}$ manifold. Under these assumptions the use of angular momentum algebra allows a straightforward derivation of the sum rules with the results described by a linear combination of tensor operators [13]. Taking the intensity measured with linearly polarized light equal to $\frac{1}{3}(I^0 + I^2)$, where I^0 and I^2 are the isotropic signal and linear dichroism, respectively, we find [e.g., by using Eq. (20) in Ref. [13]] the integrated absorption signal at the $j_{\pm}$ edge as

$$I_{j_{\pm}} = \{\tfrac{2j_{\pm}+1}{6}[\langle\underline{w}^{000}\rangle + \langle\underline{w}_0^{202}\rangle] \pm \tfrac{c}{3}[\langle\underline{w}^{110}\rangle + \tfrac{2}{5}\langle\underline{w}_0^{112}\rangle + \tfrac{3}{5}\langle\underline{w}_0^{312}\rangle]\}\,|P_{l,j_{\pm}}|^2, \tag{6}$$

where $P_{l,j_{\pm}}$ represent the radial-matrix elements of the $j_{\pm} \rightarrow l$ transitions and $\langle\underline{w}_0^{xyz}\rangle$ are the expectation values of the ground state moments in the Z direction [14]. $\underline{w}^{xyz}$ are tensor operators, where the orbital moment x and spin moment y are coupled to a total moment z. The underscore denotes that the operators act on hole states, instead of electron states, as is appropriate for XAS. Tensors with $y = 0$ are spin independent and when z is even they describe the shape of the charge distribution, i.e.,

$$\langle\underline{w}^{000}\rangle = \langle n_h\rangle, \tag{7}$$

$$\langle\underline{w}_0^{202}\rangle = \tfrac{1}{l(2l-1)}[3\langle l_z^2\rangle - l^2] \equiv \langle q_z\rangle, \tag{8}$$

give the number of holes and the quadrupole moment of the l shell, respectively. Tensors $\underline{w}^{x1z}$ describe spin-orbit correlations,

$$\langle\underline{w}^{110}\rangle = \tfrac{1}{ls}\langle l\cdot s\rangle = \tfrac{1}{3ls}\langle l_x s_x + l_y s_y + l_z s_z\rangle \equiv \langle\lambda_i\rangle, \tag{9}$$

$$\langle\underline{w}_0^{112}\rangle = \tfrac{1}{2ls}[3\langle l_z s_z\rangle - \langle l\cdot s\rangle] \equiv \tfrac{3}{2}\langle\lambda_a\rangle, \tag{10}$$

give the isotropic and anisotropic part of the spin-orbit coupling, respectively. The latter relates to the difference in probability for l and s parallel and perpendicular to the Z direction. Similarly, $\langle\underline{w}_0^{312}\rangle$ gives the coupling between the charge octupole moment and the spin moment to a total magnetic quadrupole moment. An explicit expression can be found in Refs. [11,13]. All tensors are normalized such that $\langle\underline{w}_0^{xyz}\rangle = (-1)^z$ for the magnetic ground state level $M = -J$ of the l shell containing a single hole, e.g., $d^9\,{}^2D_{5/2}(M = -5/2)$.

Intuitively, the result of Eq. (6) can be understood if we consider the sum, $\rho \equiv I_{j_+} + I_{j_-}$, and the weighed difference, $\delta \equiv I_{j_+} - \frac{c+1}{c}I_{j_-}$, of the integrated signals over the $j_{\pm}$ edges and take the radial-matrix elements equal. The sum signal, ρ, depends only on tensors with x even and $y = 0$. It gives the charge density of the unoccupied states of the l shell along the Z axis. The light acts only on the orbital part of the wave function, so that the integrated signal summed over the two edges is independent of the spin. Also by integrating over the entire spectrum we average over all possible core hole orientations, therefore the core hole properties drop out and only the ground state properties of the l shell remain. The difference signal, δ, is determined by spin-orbit coupled tensors ($y = 1$). The strong spin-orbit interaction of the core hole couples the orbital moment to the spin moment, which allow the measurement of spin dependent properties. If the total angular momentum j of the core hole is a good quantum number, we can integrate over a complete set of basis states and the core hole properties disappear. However, this criterium is only fulfilled in the absence of jj mixing, i.e., when the core-valence electrostatic interaction can be neglected with respect to the core spin-orbit interaction. If not,

there will be a transfer of spectral weight between the two j levels [10].

The sum rules have been derived for a collinear geometry, where the directions of the polarization and magnetization are parallel. For a generalization we need to include the anisotropic properties of the material. The sample can have an easy axis of magnetization, $\boldsymbol{\varepsilon}$, which is along a high-symmetry direction of the crystal lattice, and it can be magnetized in a direction $\mathbf{M}$ by an applied magnetic field. Then the expectation values of the tensors along the direction $\mathbf{P}$, which coincide with the linear polarization direction of the x rays, are given by [15]

$$\langle \underline{w}^{110} \rangle = \langle \lambda_i \rangle + \langle \lambda_a \rangle U^{220}(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}}), \tag{11}$$

$$\langle \underline{w}^{112} \rangle = \tfrac{3}{2} \langle \lambda_a \rangle U^{222}(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}}), \tag{12}$$

$$\langle \underline{w}^{202} \rangle = \langle q_z \rangle U^{202}(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}}), \tag{13}$$

$$\langle \underline{w}^{312} \rangle = \langle \underline{w}_0^{312} \rangle U^{422}(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}}), \tag{14}$$

where U^{abc} are multipole functions, which give the angular dependence with respect to the directions $\hat{\varepsilon}$, $\hat{\mathbf{M}}$, and $\hat{\mathbf{P}}$. The explicit form of these functions depends on the specific symmetry. For instance, a multilayer system homogeneous within the planes of the layers can be treated in cylindrical symmetry with Z along the surface normal. In that case $U^{220} = \frac{1}{2}[3(\hat{\varepsilon} \cdot \hat{\mathbf{M}})^2 - 1]$ and with Eq. (11) $\langle \underline{w}^{110} \rangle$ is independent of $\hat{\mathbf{P}}$. This illustrates that $c = 0$ corresponds to a monopole distribution with respect to $\hat{\mathbf{P}}$ and that $b = 2$ corresponds to a quadrupole distribution with respect to $\hat{\mathbf{M}}$. The U functions are normalized to unity for $\varepsilon \parallel \mathbf{M} \parallel \mathbf{P}$, in which case the expectation values become equal to $\langle \underline{w}_0^{xyz} \rangle$, i.e., the values along the Z direction. In the derivation of Eqs. (11)–(14) we considered only magnetic moments up to M^2 and assumed a point group symmetry higher than D_2. In lower symmetry there can be more than one quadrupole moment, which requires an extra index [15].

Generalization of Eq. (6) to include the angular dependence of Eqs. (11)–(14) gives the total signal over the $j_\pm$ edge as

$$\begin{aligned} I_{j_\pm}(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}}) = \{ & \tfrac{2j_\pm + 1}{6} [\langle n_h \rangle + \langle q_z \rangle U^{202}] \\ & \pm \tfrac{c}{3} [\langle \lambda_i \rangle + \langle \lambda_a \rangle (U^{220} + \tfrac{3}{5} U^{222}) \\ & + \tfrac{3}{5} \langle \underline{w}_0^{312} \rangle U^{422}] \} |P_{l,j_\pm}|^2 . \end{aligned} \tag{15}$$

In an arbitrary MLXD experiment we measure the difference in signal between the geometries $(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}})$ and $(\hat{\varepsilon}, \hat{\mathbf{M}}', \hat{\mathbf{P}}')$, which will lead to changes in the multipole functions equal to

$$\Delta U^{abc} = U^{abc}(\hat{\varepsilon}, \hat{\mathbf{M}}, \hat{\mathbf{P}}) - U^{abc}(\hat{\varepsilon}, \hat{\mathbf{M}}', \hat{\mathbf{P}}'). \tag{16}$$

With Eq. (15) the sum and weighted difference of the integrated signals over the $j_\pm$ edges of the MLXD spectrum are

$$\rho = \langle q_z \rangle \Delta U^{202} (\tfrac{c+1}{3} |P_{l,j_+}|^2 + \tfrac{c}{3} |P_{l,j_-}|^2), \tag{17}$$

$$\begin{aligned} \delta = & [\langle \lambda_a \rangle (\Delta U^{220} + \tfrac{3}{5} \Delta U^{222}) + \tfrac{3}{5} \langle \underline{w}_0^{312} \rangle \Delta U^{422}] \\ & \times (\tfrac{c}{3} |P_{l,j_+}|^2 + \tfrac{c+1}{3} |P_{l,j_-}|^2). \end{aligned} \tag{18}$$

When the radial-matrix elements are equal the ratio becomes

$$\frac{\delta}{\rho} = \frac{\langle \lambda_a \rangle (\Delta U^{220} + \tfrac{3}{5} \Delta U^{222}) + \tfrac{3}{5} \langle \underline{w}_0^{312} \rangle \Delta U^{422}}{\langle q_z \rangle \Delta U^{202}}, \tag{19}$$

which is generally valid for dipole transitions $c \rightarrow c + 1$, such as $s \rightarrow p$, $p \rightarrow d$, and $d \rightarrow f$.

MLXD can be measured in various ways. A common way is to keep the magnetization along the easy direction ($\mathbf{M} \parallel \varepsilon$) and to rotate the polarization direction. In cylindrical symmetry this gives $U^{ab0} = 1$ and $U^{ab2} = \frac{1}{2}[3(\hat{\varepsilon} \cdot \hat{\mathbf{P}})^2 - 1]$ so that

$$\frac{\delta}{\rho} = \frac{3}{5} \frac{\langle \lambda_a \rangle + \langle \underline{w}_0^{312} \rangle}{\langle q_z \rangle}. \tag{20}$$

Alternatively, we can keep the linear polarization along the easy direction ($\mathbf{P} \parallel \varepsilon$) but change the magnetization direction, which gives that $U^{a0c} = 1$ and $U^{a2c} = \frac{1}{2}[3(\hat{\varepsilon} \cdot \hat{\mathbf{M}})^2 - 1]$. This results in $\rho = 0$ and $\delta \propto \frac{8}{5} \langle \lambda_a \rangle + \frac{3}{5} \langle \underline{w}_0^{312} \rangle$, hence the dependence on the spin-orbit anisotropy is enhanced. The origin of this enhancement becomes clear if we consider Eq. (11) which shows that the scalar spin-orbit interaction in a magnetic material is no longer isotropic when there is a preferred magnetic orientation. This effect can be observed only upon rotation of $\mathbf{M}$ but not when $\mathbf{P}$ is rotated.

The sum rules also allow us to determine the magnitude of the MLXD signal. The atomic values of $\langle \underline{w}_0^{112} \rangle$ and $\langle \underline{w}_0^{312} \rangle$ are large (near unity, unless they vanish on symmetry grounds) which can be verified from the calculated values for transition metal compounds [16], rare earths [11], and actinides [17]. However, in metallic $3d$ systems the spin-orbit interaction is strongly reduced by the crystalline field. Furthermore, in D_4 and higher symmetry the orbital octupole moment vanishes, so that we can often neglect $\langle \underline{w}_0^{312} \rangle$.

At surfaces and interfaces the MAE can be strongly enhanced compared to bulk materials due to an increase in $\langle \lambda_a \rangle$. This can be related to a reduced coordination number which narrows the d band width and gives an enhancement of the spin moment. Furthermore, a reduction of the symmetry can change the orbital degeneracy; there can be a change in the density of states near the Fermi level; the presence of surface roughness, interdiffusion, steps, or terraces can increase the electron localization, leading to more localized atomiclike wave functions; confinement of the electronic wave function can lead to symmetry breaking and localization; and strain-induced anisotropy due to the lattice mismatch of the substrate can break the lattice symmetry of the film. An estimate of the spin-orbit anisotropy in $3d$ transition metal thin films can

be obtained by looking at the value of the orbital moment measured with MCXD. For instance, in the Au/Co/Au system Weller *et al.* [4] found an anisotropy in the Co $3d$ orbital moment of $\sim 0.1 \mu_B$. Assuming that all d holes are in the minority spin band, this yields $\langle \lambda_a \rangle \approx 0.05$.

The branching ratio, $\mathcal{B} = I_{j_+}/(I_{j_+} + I_{j_-})$, provides a useful way to monitor small changes in $\langle \lambda \rangle$. Equation (15) yields

$$\mathcal{B} \approx \mathcal{B}_0 + (1 - \mathcal{B}_0)\langle \lambda \rangle / \langle n_h \rangle , \qquad (21)$$

where $\mathcal{B}_0$ is the statistical value, which is equal to $(c + 1)/(2c + 1)$ when j is a good quantum number. Even when the value of $\mathcal{B}_0$ is modified due to core-valence interaction, Eq. (21) can still be applied to determine $\langle \lambda \rangle$ [10]. Changes in the branching ratio in the order of a percent should be easily observable. The increased photon flux of next generation synchrotron radiation devices will push this detection limit even further down. Imaging of magnetic domain structures with linearly polarized x rays will allow us to obtain information on a microscopic scale. The explicit dependence on the spin-orbit coupling makes it also possible to separate the MAE from macroscopic magnetic orientation effects, such as the shape anisotropy. This is of importance for the understanding of phenomena such as PMA.

We note that for spectra taken with circularly polarized x rays the branching ratio is [13]

$$\mathcal{B}_\pm \approx \mathcal{B}_0 \pm (1 - \mathcal{B}_0)\langle S_z \rangle / \langle n_h \rangle , \qquad (22)$$

where the $\pm$ sign refers to an alignment with the light helicity and magnetization parallel and antiparallel, respectively. Comparison with Eq. (21) shows that the MLXD signal will generally be much smaller than the MCXD, especially for ferromagnetic materials, such as Fe, Co, and Ni.

Although the original derivation of the sum rules is based on an atomic approach, there have been several theoretical and experimental studies indicating that the MCXD-sum rules can also be applied to metallic systems [18,19]. Since the spin-orbit coupling is a local interaction, the extension to metals should certainly hold for MLXD.

Equation (19) can also be used to analyze the linear dichroism in the d core spectra of lanthanides and actinides. If the crystal field interaction in the f shell is small compared to the spin-orbit interaction, which is often the case, then according to the Wigner-Eckart theorem the operators with the same z are proportional to each other and their moments are aligned parallel [17]. Thus for small crystal fields the ratio ρ/δ depends only on the Coulomb interaction and spin-orbit coupling. It is further interesting to note that for the Hund's rule ground state of the f^n configuration, $\langle \underline{w}^{312} \rangle = 0$ for $n =$ 2, 5, 6, 7, 9, and 12 [17].

Summarizing, we demonstrated that the sum and weighted difference signals over the $j_\pm$ edges in the MLXD spectrum are proportional to the anisotropy in the charge distribution and spin-orbit interaction, respectively. Because the latter is directly related to the MAE, MLXD can become a valuable tool to measure the magnetocrystalline anisotropy energy of thin films and multilayers in an element-specific and laterally resolved manner.

[1] J. H. van Vleck, Phys. Rev. **52**, 1178 (1937).
[2] L. Néel, J. Phys. Radium **15**, 376 (1954).
[3] P. Bruno, Phys. Rev. B **39**, 865 (1989).
[4] D. Weller, J. Stöhr, R. Nakajima, A. Carl, M. G. Samant, C. Chappert, R. Mégy, P. Beauvillain, P. Veillet, and G. Held, Phys. Rev. Lett. **75**, 3752 (1995).
[5] G. van der Laan, B. T. Thole, G. A. Sawatzky, J. B. Goedkoop, J. C. Fuggle, J. M. Esteva, R. C. Karnatak, J. P. Remeika, and H. A. Dabkowska, Phys. Rev. B **34**, 6529 (1986).
[6] P. Kuiper, B. G. Searle, P. Rudolf, L. H. Tjeng, and C. T. Chen, Phys. Rev. Lett. **70**, 1549 (1993).
[7] J. Vogel and M. Sacchi, Phys. Rev. B **49**, 3230 (1994); **53**, 3409 (1996).
[8] M. M. Schwickert, G. Y. Guo, M. A. Tomaz, W. L. O'Brien, and G. R. Harp, Phys. Rev. B **58**, R4289 (1998).
[9] D. S. Wang, R. Wu, and A. J. Freeman, Phys. Rev. B **47**, 14 932 (1993).
[10] B. T. Thole and G. van der Laan, Phys. Rev. B **38**, 3158 (1988); Phys. Rev. A **38**, 1943 (1988).
[11] P. Carra, H. König, B. T. Thole, and M. Altarelli, Physica (Amsterdam) **192B**, 182 (1993).
[12] J. Luo, G. T. Trammell, and J. P. Hannon, Phys. Rev. Lett. **71**, 287 (1993).
[13] G. van der Laan, Phys. Rev. B **57**, 112 (1998).
[14] G. van der Laan and B. T. Thole, J. Phys. Condens. Matter **7**, 9947 (1995), Appendix A.
[15] G. van der Laan, Phys. Rev. B **57**, 5250 (1998).
[16] G. van der Laan and B. T. Thole, Phys. Rev. B **43**, 13 401 (1991).
[17] G. van der Laan and B. T. Thole, Phys. Rev. B **53**, 14 458 (1996).
[18] R. Wu, D. Wang, and A. J. Freeman, Phys. Rev. Lett. **71**, 3581 (1993); R. Wu and A. J. Freeman, Phys. Rev. Lett. **73**, 1994 (1994); A. Ankudinov and J. J. Rehr, Phys. Rev. B **51**, 1282 (1995).
[19] C. T. Chen, Y. U. Idzerda, H.-J. Lin, N. V. Smith, G. Meigs, E. Chaban, G. H. Ho, E. Pellegrin, and F. Sette, Phys. Rev. Lett. **75**, 152 (1995).